

Charge-density-wave phases of the generalized t - V model

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The one-dimensional extended t - V model of fermions on a lattice is a model with repulsive interactions of finite range that exhibits a transition between a Luttinger liquid conducting phase and a Mott insulating phase. It is known that by tailoring the potential energy of the insulating system, one can force a phase transition into another insulating phase. We show how to construct all possible charge-density-wave phases of the system at low critical densities in the atomic limit. Higher critical densities are investigated by a brute-force analysis of the possible finite unit cells of the Fock states.

I. INTRODUCTION

Low-dimensional quantum systems exhibit unique electronic properties impossible to realize in bulk. A proper theoretical understanding of these materials could allow us to use them in a variety of novel electronic devices. Many low-dimensional systems show interesting behavior, such as the presence of phases that cannot be explained using classical theory.¹ One example of such phases is a Mott insulator, which has applications ranging from high-temperature superconductors² to a new type of energy-efficient field effect transistor with fast switching times.³ The research into the subject of one- and two-dimensional Mott transistors is currently ongoing.^{4–6} However, to make an efficient Mott insulating device we first need an accurate description of the possible phase diagram of the system.

All one-dimensional quantum liquids fall into the universality class of a Luttinger liquid,^{1,7–9} which is a concept similar to the Fermi liquid in higher dimensions. The theory of Luttinger liquids has already proven to be applicable in experiments dealing with carbon nanotubes,¹⁰ the fractional quantum Hall effect,^{11,12} and crystals of trapped ions.¹³

The extended t - V model¹⁴ is a perfect subject for investigation, exhibiting both a conducting Luttinger liquid phase and a Mott insulator phase. Recent studies^{15–18} have shown that one can achieve multiple insulating quantum phases in this system and thus there is a question of how to provide a systematic description of these insulators when the interaction range is varied.

In this article we investigate charge-density-wave (CDW) insulating phases that are present in a system with specific potential energy. The outline of this work is as follows: in Sec. II we present a generalization of the t - V model and describe its known behavior; then in Sec. III we investigate CDW phases at low critical densities, while higher critical densities are analyzed in Sec. IV using brute-force sampling of the partial basis; finally, in Section V we conclude and discuss possible future work.

II. THE GENERALIZED t - V MODEL

The Hamiltonian of the generalized t - V model of spinless fermions in a one-dimensional periodic chain of length L is given by^{14,19}

$$\hat{H} = -t \sum_{i=1}^L (\hat{c}_i^\dagger \hat{c}_{i+1} + \text{h.c.}) + \sum_{i=1}^L \sum_{m=1}^p U_m \hat{n}_i \hat{n}_{i+m}, \quad (1)$$

where \hat{c}_i and \hat{c}_i^\dagger are the fermionic annihilation and creation operators on site i , $\hat{n}_i = \hat{c}_i^\dagger \hat{c}_i$ is the particle number operator, p is the maximum range of the interaction, t is the strength of the kinetic energy, and $U_m \geq 0$ is the potential between two fermions that are m sites apart from each other (for $m > p$, $U_m = 0$). Notice that the potential part is diagonal in the basis consisting of Fock states.

The hopping part is assumed to have much smaller strength than the potential part, i.e., $\forall_{m \leq p} t \ll U_m$, which means that two fermions are likely to be more than p sites away from each other. This also leads to a critical Mott insulating density $Q = \frac{1}{p+1}$, where there is a huge energy penalty to moving any one fermion. By shaking a system in the critical density, one can create a CDW. Gómez-Santos¹⁴ introduces another very important assumption:

$$\forall_m U_m < \frac{U_{m+1} + U_{m-1}}{2}. \quad (2)$$

If the fermion-fermion distance is required to be less than p sites (due to high density in the system), then the particles will want to be as spread out as possible. One can for example consider two similar systems, both in Fock states, which are different only by fermion chains: $(\dots \bullet \bullet \bullet \bullet \bullet \bullet \dots)$ and $(\dots \bullet \bullet \bullet \bullet \bullet \bullet \dots)$, where \bullet and \circ denote occupied and empty sites respectively. Assumption (2) tells us that the first system will always have lower energy regardless of the maximum range of interactions. Thus, there are critical densities $Q = \frac{1}{m}$, when $m = 1, 2, \dots, p+1$, at which the system is insulating and has the following unperturbed ($t \rightarrow 0$) ground state:

$$\underbrace{\bullet \circ \circ \circ \circ \circ}_{1/Q-1} \underbrace{\bullet \circ \circ \circ \circ \circ}_{1/Q-1} \underbrace{\bullet \circ \circ \circ \circ \circ}_{1/Q-1} \dots \quad (3)$$

sites

and the energy density is $EQ/N = QU_{1/Q}$ if $m > \frac{p+1}{2}$, where $N = \sum_i \hat{n}_i$ is the total number of particles in the system. By converting condition (2) into

$$\bigvee_m \frac{U_{m+1} + U_{m-1} - 2U_m}{a^2} > 0, \quad (4)$$

where a is the lattice constant, we can immediately see that this assumption is a discrete version of the (continuous) inequality

$$U''(r) > 0. \quad (5)$$

One can easily check that assumption (5) holds for Coulomb and dipole potentials. However, in principle, a potential that does not satisfy such a condition could also be considered (such as the Pöschl-Teller potential used in the description of ultracold atomic gases).

Models with interaction range $p = 2$ and $Q = 1/3$ and $1/2$ have already been analyzed in Refs. 15 and 16. Depending on the strength of the potentials, one can have different phases in the system: there can be multiple CDW insulating phases, a long-range bond-order phase, and even a Luttinger liquid phase, despite the existence of a critical (“insulating”) density.

The objective of this work is to generalize this result for all interaction ranges. However, to simplify the problem, we shall assume the atomic limit ($t = 0$), in which the only phases that will be encountered are CDW insulators.

III. LOW CRITICAL DENSITIES IN THE ATOMIC LIMIT

A. Critical density $Q = 1/(p+1)$

In the trivial case of $Q = 1/(p+1)$, the ground-state energy is always equal to zero. The ground-state configuration is

$$\bullet \underbrace{\circ \circ \dots \circ}_p \bullet \underbrace{\circ \circ \dots \circ}_p \bullet \underbrace{\circ \circ \dots \circ}_p \dots \quad (6)$$

$$\boxed{\underbrace{\bullet \underbrace{\circ \circ \dots \circ}_{p-n} \bullet \underbrace{\circ \circ \dots \circ}_p \bullet \underbrace{\circ \circ \dots \circ}_p \bullet \underbrace{\circ \circ \dots \circ}_p \dots}_{n-1 \text{ times}}} \dots, \quad (9)$$

with the energy $E_n = \frac{L}{1+p-n+(n-1)(p+1)} U_{p+1-n} = \frac{L}{np} U_{p-n+1} = \frac{N}{n} U_{p-n+1}$. We can now calculate the exact conditions in which an arbitrary phase (designated by step n) will be dominant in the system:

$$\begin{aligned} \bigvee_{k \neq n} E_n &< E_k \\ \Rightarrow \bigvee_{k \neq n} U_{p-n+1} &< \frac{n}{k} U_{p-k+1}. \end{aligned} \quad (10)$$

Such a ground state is $(p+1)$ -fold degenerate since the energy is invariant under translation.

B. Critical density $Q = 1/p$

Let us now show how to construct the CDW phase for a system with any p and with critical density $Q = \frac{1}{p}$. Firstly, assume that U_p is low enough to ensure that the preferable distance between two fermions is always p and thus we can say that U_p orders the fermions in the ground state; for example a chain $\bullet \underbrace{\circ \circ \dots \circ}_{p-1} \bullet \underbrace{\circ \circ \dots \circ}_{p-1} \bullet$ has lower energy than $\bullet \underbrace{\circ \circ \dots \circ}_p \bullet \underbrace{\circ \circ \dots \circ}_{p-2} \bullet$. The ground state must have the simple form

$$\bullet \underbrace{\circ \circ \dots \circ}_{p-1} \bullet \underbrace{\circ \circ \dots \circ}_{p-1} \bullet \underbrace{\circ \circ \dots \circ}_{p-1} \dots \quad (7)$$

and its energy is $E_1 = \frac{L}{p} U_p = N U_p$.

Now, let us assume that U_{p-1} is low enough to order the fermions. We could use a series of $\bullet \underbrace{\circ \circ \dots \circ}_{p-2} \bullet$ sections, but then we would not achieve the correct density $1/p$. However, by addition of sections $\bullet \underbrace{\circ \circ \dots \circ}_p \bullet$ we can tailor the density without changing the energy of the system. Thus, the ground-state configuration is

$$\boxed{\bullet \underbrace{\circ \circ \dots \circ}_{p-2} \bullet \underbrace{\circ \circ \dots \circ}_p \bullet \underbrace{\circ \circ \dots \circ}_{p-2} \bullet \underbrace{\circ \circ \dots \circ}_p \bullet \underbrace{\circ \circ \dots \circ}_{p-2} \bullet \underbrace{\circ \circ \dots \circ}_p \bullet \dots}_{n-1 \text{ times}}, \quad (8)$$

which gives us the correct density $Q = \frac{2}{2p} = \frac{1}{p}$ and energy $E_2 = \frac{L}{2p} U_{p-1} = \frac{N}{2} U_{p-1}$. The boxes are present to show that we have correctly counted the energy and particle density. In general, however, the whole subspace of the unperturbed ground states would include Fock states in which sections with $p-2$ holes could be beside each other, unless they would change the energy of the system.

If one follows this prescription, in the n -th step the following ground state is obtained:

Renaming $\alpha = p - n + 1$ and $\beta = p - k + 1$,

$$\bigvee_{\beta \neq \alpha} U_\alpha < \frac{p - \alpha + 1}{p - \beta + 1} U_\beta. \quad (11)$$

If this condition is fulfilled, then the phase with energy $E_{(\alpha)} = \frac{N}{p-\alpha+1} U_\alpha$ is dominant and the ground state consists of $\frac{N}{p-\alpha+1}$ blocks of $\bullet \underbrace{\circ \circ \dots \circ}_{\alpha-1} \bullet$ and $N \frac{p-\alpha}{p-\alpha+1}$ blocks of $\bullet \underbrace{\circ \circ \dots \circ}_p \bullet$.

$\bullet \underbrace{\circ \circ \dots \circ}_p$ and is f -fold degenerate, where:

$$f = \begin{cases} \binom{N}{N/(p-\alpha+1)} \cdot p & \text{if } 2\alpha > p \\ \binom{N \frac{p-\alpha}{p-\alpha+1}}{N/(p-\alpha+1)} \cdot \frac{p(p-\alpha+1)}{p-\alpha} & \text{otherwise.} \end{cases} \quad (12)$$

For $2\alpha \leq p$ the problem with assessing the degeneracy is that we need to exclude cases where blocks of $\bullet \underbrace{\circ \circ \dots \circ}_{\alpha-1}$ are too close to each other and thus would increase the energy by $U_{2\alpha}$.

IV. HIGHER CRITICAL DENSITIES IN THE ATOMIC LIMIT

For Mott insulators with $Q = \frac{1}{m}$, where $m = 1, \dots, p-1$, the number of phases and their energies were found to be more difficult to obtain. Rather than constructing the phases as done in Section III, we shall use a brute-force analysis of the basis for systems of finite size. Nevertheless, because we are interested in the thermodynamic limit, a periodic system of L sites can be thought of as an infinite system with a unit cell of L sites.

A. Properties of the system

Sampling the full basis in systems with $Q > 1/p$ is problematic, because the dimension of the basis grows rapidly with a system size. However, many of the Fock states will have the same energy. In particular, if two states are cyclic permutations of each other, or cyclic permutations with inversion, then such states must have the same energy due to the periodicity of the system. Checking the full basis for cyclic permutations would still be computationally quite a difficult task: firstly, because generating the full basis would take a lot of memory, and secondly, because comparing all the states to check if they are cyclic permutations would require a large computational time [of $O(2^{2L})$]. An alternative approach to this problem is to consider the spaces between the fermions in our chain and to develop rules to generate a set of Fock states that will always contain ground states of the system.

Theorem 1 *For any basis state, the largest space between consecutive fermions must not be less than $1/Q - 1$ sites.*

Proof. All spaces between consecutive fermions are equal only if all particles are $1/Q - 1$ sites apart, i.e., the configuration is

$$\bullet \underbrace{\circ \circ \dots \circ}_{1/Q-1} \bullet \underbrace{\circ \circ \dots \circ}_{1/Q-1} \dots \bullet \underbrace{\circ \circ \dots \circ}_{1/Q-1} \bullet \quad (13)$$

Any attempt to move a fermion would make the largest space bigger than $1/Q - 1$. ■

Thus, any state will have a space that is larger than or equal to $1/Q - 1$. Due to the system's periodicity, we can therefore fix the first $1/Q$ sites to be

$$\bullet \underbrace{\circ \circ \dots \circ}_{1/Q-1} \bullet \quad (14)$$

This leaves us with a smaller subspace of the full basis to generate: the system with size $(N-1)/Q$ and $N-1$ particles.

Theorem 2 *For any ground state of the system, the largest space must not exceed p sites.*

Proof. Assume that there exists a ground state unit cell with the largest space equal to $p+1$ sites. We can write it as

$$\underbrace{\bullet ?? \dots ? \bullet \circ \circ \dots \circ}_p \quad (15)$$

Let E_A be the energy of the block A , so that the energy density of this ground state is $\frac{E_A}{N/Q}$. Let us construct the following unit cell, which consists of p consecutive ground-state unit cells (15):

$$\underbrace{\underbrace{\bullet ?? \dots ? \bullet \circ \circ \dots \circ}_p \underbrace{\bullet ?? \dots ? \bullet \circ \circ \dots \circ}_p \dots \underbrace{\bullet ?? \dots ? \bullet \circ \circ \dots \circ}_p}_p \quad (16)$$

This unit cell has the same energy density $\frac{pE_A}{pN/Q} = \frac{E_A}{N/Q}$ as the ground-state unit cell (15). Let us now move the additional empty spaces to the end of this chain, which still does not change the energy density:

$$\underbrace{\bullet ?? \dots ? \bullet \circ \circ \dots \circ}_p \underbrace{\bullet ?? \dots ? \bullet \circ \circ \dots \circ}_p \dots \underbrace{\bullet ?? \dots ? \bullet \circ \circ \dots \circ \circ \circ \dots \circ}_p \quad (17)$$

Now, let us assume that the last fermion in block A contributes to the potential energy of this block by amount E_Δ . If $E_\Delta = 0$, we can always swap this last fermion with the rest of block A and again consider the last fermion of a new block. If we take this last fermion out and replace it with a hole, then the energy of the block A will decrease by E_Δ . Let us now move the last fermion in unit cell (17) by p sites to the right:

$$\underbrace{\bullet ?? \dots ? \bullet \circ \circ \dots \circ}_p \underbrace{\bullet ?? \dots ? \bullet \circ \circ \dots \circ}_p \dots \underbrace{\bullet ?? \dots ? \circ \circ \dots \circ \bullet \circ \circ \dots \circ}_{p-1} \underbrace{\circ \circ \dots \circ}_p, \quad (18)$$

where block A' is block A with the last fermion replaced by a hole. Block A' has energy $E_A - E_\Delta$. The last fermion does not contribute now to the overall potential energy, because it is surrounded by p sites on both sides. Such a unit cell now has energy density

$$\frac{pE_A - E_\Delta}{pN/Q} = \frac{E_A}{N/Q} - \frac{E_\Delta}{pN/Q}, \quad (19)$$

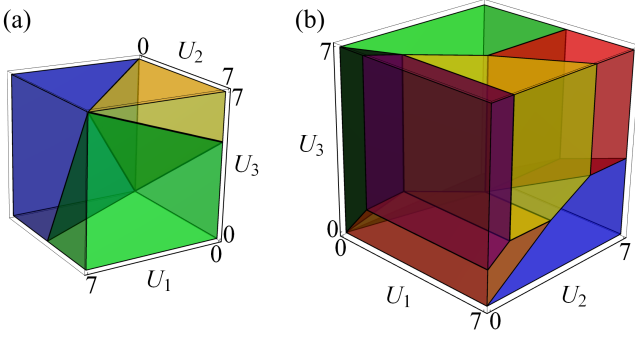


FIG. 1. (Color online) Phase diagrams of (a) $p = 3, Q = 1/2$ and (b) $p = 4, Q = 1/3$ with $U_4 = 1$. For color legend see Table I.

which is lower than the energy of the ground-state unit cell (15), and this leads to a contradiction. A similar process can be used to show that a ground state cannot have a space equal to $p + 2$ and more sites. Thus, we conclude that the largest space in any ground state must have at most p sites. ■

Using Theorems 1 and 2, we can significantly decrease the number of generated states.

B. Details of the calculations

Our calculations were performed using Mathematica.²⁰ Firstly a partial basis for a specific number of particles N , density Q and interaction range p was generated. States of this partial basis had the first $1/Q$ sites fixed to the configuration shown in Eq. (14) by Theorem 1, and any states that were not in agreement with Theorem 2 were removed. Then, the energy density was calculated²¹ for every state and this list of energies was simplified by removing duplicates. In order to discard the energies that cannot describe the ground state, the expression $\forall_\beta E_\alpha < E_\beta$ was assessed²². Some energies however could not be compared without knowing the values of $\{U_m\}$. The final list contains the energies of all phases that have the lowest energy for some set values of $\{U_m\}$; these are the CDW phases of the system.

C. Results for $Q = 1/(p - 1)$

Unit cells and energy densities for $p = 3, 4$, and 5 are presented in Table I. Due to the finite size of the systems studied, we can only look for CDW unit cells up to a specific size (L_{\max}). Phase diagrams in Figure 1 show what phases are expected to appear for different values of the potentials $\{U_m\}$.

TABLE I. Ground-state (GS) unit cells and their energies in a system with $Q = 1/(p - 1)$. f is the degeneracy of the ground state. L_{\max} is the maximum size of the unit cell that was analyzed. Colors designate phases shown in Fig. 1 (color online).

System	GS unit cell	Energy density	f
$p = 3,$	●○	$\frac{1}{2}U_2$	2 ■
$Q = 1/2,$	●●○○	$\frac{1}{4}(U_1 + U_3)$	4 ■
$L_{\max} = 28$	●●●○○○	$\frac{1}{6}(2U_1 + U_2)$	6 ■
$p = 4,$	●○○	$\frac{1}{3}U_3$	3 ■
$Q = 1/3,$	●●○○○○	$\frac{1}{6}U_1$	6 ■
$L_{\max} = 36$	●●●○○○	$\frac{1}{6}(U_2 + U_4)$	6 ■
	●●○○○●○○○	$\frac{1}{9}(U_1 + 2U_4)$	9 ■
	●○○●○○○○	$\frac{1}{9}(2U_2 + U_4)$	9 ■
	●○●○○○●○○○○	$\frac{1}{12}(2U_2 + U_3)$	12 ■
	●●○○○○●○●○○○○●○○○○●○○○○	$\frac{1}{31}(2U_1 + 3U_2)$	21 ■
$p = 5,$	●○○○	$\frac{1}{4}U_4$	4
$Q = 1/4,$	●○○●○○○	$\frac{1}{8}(U_3 + U_5)$	8
$L_{\max} = 32$	●○○●○○○	$\frac{1}{8}U_2$	8
	●○●○○○●○○○○	$\frac{1}{12}(U_2 + 2U_5)$	12
	●○○●○○●○○○○	$\frac{1}{12}2U_3$	12
	●●○○○○●○○○○●○○○○	$\frac{1}{16}(U_1 + 3U_5)$	16
	●●○○○○●●○○○○●○○○○○	$\frac{1}{20}2U_1$	20

D. Results for $Q = 1/(p - 2)$

Table II presents the unit cells and energy densities for $p = 4$ and 5 . Notice that for $p = 5$, we have found ground-state unit cells up to L_{\max} and thus potentially there could be a ground state containing an even larger unit cell that was not found in our calculation.

E. Discussion of the results

Our results illustrate how highly nontrivial and unpredictable the ground-state configurations are for critical densities higher than $Q = 1/p$. For example, for a half-filled system ($Q = 1/2$), judging only from the $p = 3$ case, one would naively expect a similar trend to be present in all other cases: for all units cells to consist of a chain of occupied sites, followed by a chain of the same length, but with empty sites. However, Table II shows that for $p = 4$ there exists a ground state with a unit cell (●●○○●○○), which does not follow this prediction. Therefore, it is very difficult to create a simple set of rules describing the ground-state properties of all the phases in the system with high critical density.

We also conclude that the number of possible CDW phases in the system grows with the maximum interaction range p and the density Q . For example, in the system $p = 5, Q = 1/3$ presented in Table II, there

TABLE II. As Table I, but for a system with density $Q = 1/(p-2)$.

GS unit cell	Energy density	f
$p = 4, Q = 1/2, L_{\max} = 26$		
•○	$\frac{1}{2}(U_2 + U_4)$	2
••○○	$\frac{1}{4}(U_1 + U_3 + 2U_4)$	4
•••○○○	$\frac{1}{6}(2U_1 + U_2 + U_4)$	6
••••○○○○	$\frac{1}{8}(3U_1 + 2U_2 + U_3)$	8
•••○○○•○	$\frac{1}{8}(U_1 + 2U_2 + 3U_3)$	8
$p = 5, Q = 1/3, L_{\max} = 21$		
•○○	$\frac{1}{3}U_3$	3
•○○○○	$\frac{1}{6}(U_2 + U_4)$	6
••○○○○	$\frac{1}{6}(U_1 + U_5)$	6
••○○○○○○	$\frac{1}{9}(U_1 + U_2 + U_3)$	2×9
••○○○•○○	$\frac{1}{9}(U_1 + 2U_4 + 2U_5)$	9
•○○•○○○○	$\frac{1}{9}(2U_2 + U_4 + U_5)$	9
•○○○○•○○○○	$\frac{1}{12}(2U_2 + U_3 + 3U_5)$	12
••○○○○○○○○○○	$\frac{1}{15}(U_1 + 2U_3 + 4U_4)$	15
••○○○○○○•○○○○	$\frac{1}{15}(2U_1 + 2U_2 + U_5)$	2×15
••○○○○○○•○○○○○	$\frac{1}{15}(3U_1 + U_2)$	15
••○○•○○○○○○○○○○	$\frac{1}{18}(3U_1 + U_3 + 2U_4 + U_5)$	18
••○○○○○○•○○○○○○	$\frac{1}{18}(2U_1 + 3U_2 + U_4)$	18
••○○○○○○○○○○○○○○○○	$\frac{1}{21}(3U_1 + 2U_3 + 2U_4)$	21
••○○○○○○•○○○○○○○○○○	$\frac{1}{21}(2U_1 + 3U_2 + 3U_5)$	21

are at least 14 different CDW phases, and we expect $p = 6, Q = 1/4$ to contain even more.

For $t \neq 0$, we expect non-CDW phases to be present in the system. If one considers the phase diagrams from Fig. 1, on the interfaces between any two phases there probably are Luttinger liquid and bond-order phases, similarly to the findings of Refs. 15 and 16. Therefore, if

our assumption that the number of phases grows quickly with the maximum interaction range is correct, then we can predict that for high p , the phase diagram consists of mainly non-CDW phases, while CDW insulators are only present when certain U_m are very high. Thus, a large interaction range may imply the loss of insulating properties of the material.

V. SUMMARY AND OUTLOOK

We have studied the ground-state properties of the extended t - V model on a lattice with a potential that does not necessarily satisfy Eq. (2). We have shown how to construct the ground state of all the Mott insulating phases at low critical densities, and we have calculated the ground-state unit cells of a few example cases for higher critical densities. Thus, we provide a description of possible CDW phases of the system with any interaction range and any critical density in the atomic limit.

One could also work beyond the atomic limit ($t > 0$), in which case other, non-CDW phases would be present in the system. However, to find a simple description of all the phases while varying the interaction range could prove to be more difficult. To simulate such systems, we propose to use matrix product states^{23,24}, due to their recent achievements in calculations of lattice models using relatively low resources.

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- ²¹ Instead of using loop statements to fill in tables, it was found that the Mathematica's `Table[]` function was more efficient and the time consumption scaled exactly exponentially with the system size.
- ²² Mathematica's `Reduce[]` function was found to give the most reliable simplification results, however it also needed much higher computational resources. `Simplify[]` and `FullSimplify[]` were found to be quite similar in resource consumption and the latter was chosen due to higher reliability for simplifying complicated conditions.
- ²³ D. Perez-Garcia, F. Verstraete, M. M. Wolf, and J. I. Cirac, Quantum Inf. Comput. **7**, 401 (2007).
- ²⁴ F. Verstraete, V. Murg, and J. Cirac, Adv. Phys. **57**, 143 (2008).